=> d his

(FILE 'HOME' ENTERED AT 10:16:56 ON 11 APR 2005)

FILE 'CAPLUS' ENTERED AT 10:17:44 ON 11 APR 2005
E US6624197/PN
L1 4 S E3
SELECT RN L1 1

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L2 10 S E1-E10

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L3 STRUCTURE UPLOADED
L4 1 S L3
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L6 11 S L5

=> d l3
L3 HAS NO ANSWERS
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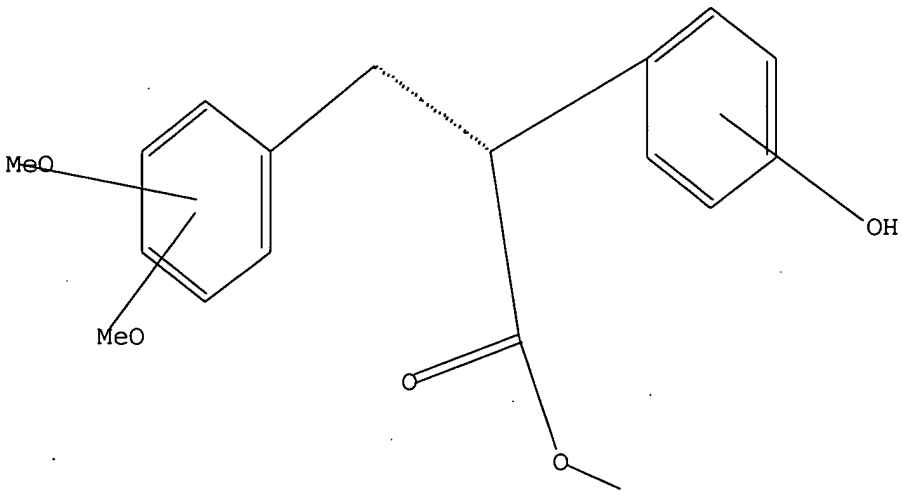


Structure attributes must be viewed using STN Express query preparation.

=> d bib abs hitstr 1-11

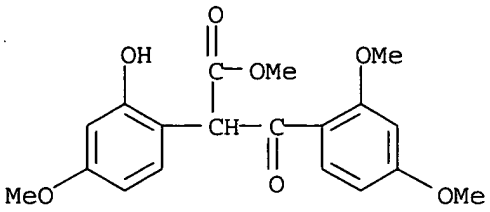
L6 ANSWER 1 OF 11 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2004:75190 CAPLUS
DN 140:321127
TI A new short synthesis of coumestrol and its application for the synthesis of [6,6a,11a-13C3]coumestrol
AU Al-Maharik, Nawaf; Botting, Nigel P.
CS School of Chemistry, University of St Andrews, St Andrews, Fife, KY16 9ST, UK
SO Tetrahedron (2004), 60(7), 1637-1642
CODEN: TETRAB; ISSN: 0040-4020
PB Elsevier Science B.V.
DT Journal
LA English
AB A convenient and simple two-step method for the synthesis of coumestrol

has been established, which involves a base catalyzed condensation of Ph acetate with benzoyl chloride, followed by demethylation and subsequent tandem intramol. cyclization. This method was then employed for the efficient synthesis of multiply 13C-labeled coumestrol.

IT **677717-62-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of coumestrol and [6,6a,11a-13C3]coumestrol)

RN 677717-62-3 CAPLUS

CN Benzenepropanoic acid, α-(2-hydroxy-4-methoxyphenyl)-2,4-dimethoxy-β-oxo-, methyl ester (9CI) (CA INDEX NAME)



RE.CNT 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2003:757334 CAPLUS

DN 139:276885

TI Preparation of novel heterocyclic analogs of diphenylethylene compounds as antidiabetics

IN Neogi, Partha; Dey, Debendranath; Medicherla, Satyanarayana; Nag, Bishwajit; Lee, Arthur

PA USA

SO U.S. Pat. Appl. Publ., 66 pp., Cont.-in-part of U.S. Ser. No. 843,167.
CODEN: USXXCO

DT Patent

LA English

FAN.CNT 9

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2003181494	A1	20030925	US 2002-265902	20021008
	US 2002025975	A1	20020228	US 2001-785554	20010220
	US 2002032225	A1	20020314	US 2001-843167	20010427
	WO 2004033438	A1	20040422	WO 2003-US31803	20031008
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
PRAI	US 1999-287237	A2	19990406		
	US 2000-591105	B2	20000609		
	US 2001-785554	A2	20010220		
	US 2001-843167	A2	20010427		
	US 1998-74925	A2	19980508		
	US 2002-265902	A2	20021008		

OS MARPAT 139:276885

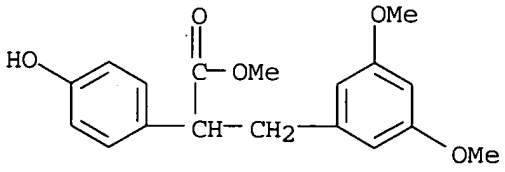
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The title compds. [I; Z = II-IV; n, m, q and r = 0-4 (n+m ≤ 4 and q+r ≤ 4); p, s = 0-5 (p+s ≤ 5); R, R2 = H, alkyl, alkenyl, etc.; R1 = H, alkyl, alkenyl, etc.; A, A1, A2 = H, acylamino, acyloxy, alkanoyl, etc.; B, B1, B2 = H, acylamino, acyloxy, alkanoyl, etc.; or A and B together, or A1 and B1 together, or A2 and B2 together, may be joined to form a methylenedioxy or ethylenedioxy; X, X1 = (un)substituted NH, O, S] which are effective in lowering blood glucose level, serum insulin, triglyceride and free fatty acid levels in animal models of Type II diabetes, were prepared E.g., a multi-step synthesis of V, starting from 3,5-dimethoxybenzaldehyde and 4-hydroxyphenylacetic acid, was given. The compound V showed strong glucose lowering activity even though it is a weak PPAR-γ agonist (data given). The compds. I are disclosed as useful for a variety of treatments including the treatment of inflammation, inflammatory and immunol. diseases, insulin resistance, hyperlipidemia, coronary artery disease, cancer and multiple sclerosis. Pharmaceutical composition comprising the compound I was claimed.

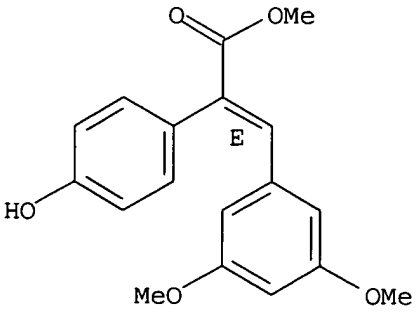
IT **380881-43-6P 606932-78-9P 606932-85-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of diphenylethylene compds. containing thiazolidinedione or oxazolidinedione moieties for treating diabetes, inflammatory or immunol. disease in combination with other agents)

RN 380881-43-6 CAPLUS
CN Benzenepropanoic acid, α-(4-hydroxyphenyl)-3,5-dimethoxy-, methyl ester (9CI) (CA INDEX NAME)



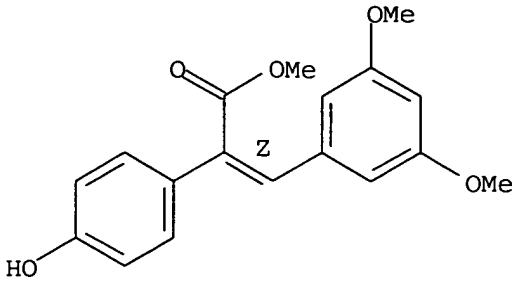
RN 606932-78-9 CAPLUS
CN Benzeneacetic acid, α-[(3,5-dimethoxyphenyl)methylene]-4-hydroxy-, methyl ester, (αE)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

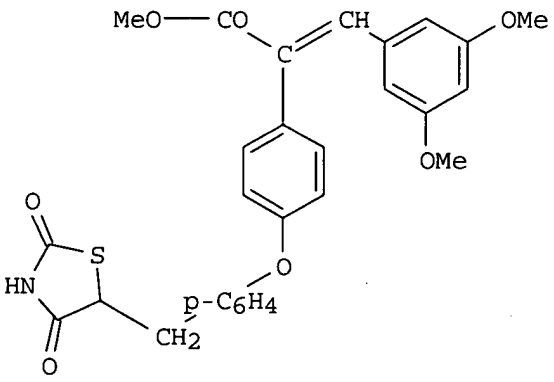


RN 606932-85-8 CAPLUS
CN Benzeneacetic acid, α-[(3,5-dimethoxyphenyl)methylene]-4-hydroxy-, methyl ester, (αZ)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L6 ANSWER 3 OF 11 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2003:645701 CAPLUS
DN 140:87046
TI Synthesis and structure-Activity relationship studies of cinnamic acid-based novel thiazolidinedione antihyperglycemic agents
AU Neogi, Partha; Lakner, Fredrick J.; Medicherla, Satyanarayana; Cheng, Jin; Dey, Debendranath; Gowri, Maya; Nag, Bishwajit; Sharma, Somesh D.; Pickford, Lesley B.; Gross, Coleman
CS Department of Chemistry, Calyx Therapeutics Inc., Hayward, CA, 94545, USA
SO Bioorganic & Medicinal Chemistry (2003), 11(18), 4059-4067
CODEN: BMECEP; ISSN: 0968-0896
PB Elsevier Science Ltd.
DT Journal
LA English
OS CASREACT 140:87046
GI

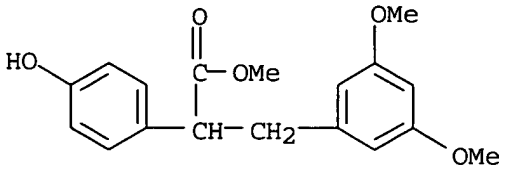


I

AB A number of 2,4-thiazolidinedione derivs. of -Ph substituted cinnamic acid were synthesized and studied for their PPAR agonist activity. The E-isomer of cinnamic acid, I, showed moderate PPAR transactivation. The corresponding Z-isomer and double bond reduced derivative were found to be much less potent. Although the E-isomer showed a moderate PPARγ transactivation, it demonstrated a strong glucose-lowering effect in a genetic rodent model of diabetes. Results of pharmacokinetic, metabolism and permeability studies are consistent with I being an active prodrug with the hydrolyzed carboxylate as an active metabolite that has similar glucose lowering and PPARγ agonist properties.
IT **380881-43-6P 606932-78-9P 606932-85-8P**

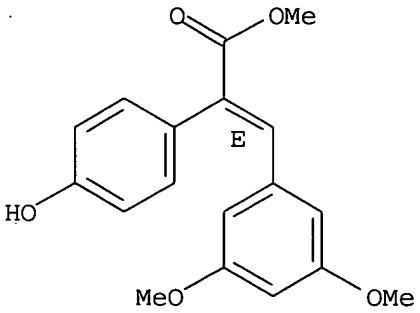
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(cinnamic acid-based thiazolidinedione antihyperglycemic agents)

RN 380881-43-6 CAPLUS
CN Benzenepropanoic acid, α-(4-hydroxyphenyl)-3,5-dimethoxy-, methyl ester (9CI) (CA INDEX NAME)



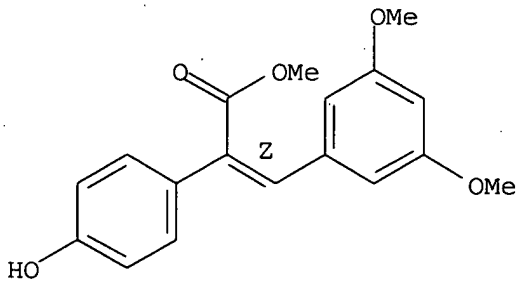
RN 606932-78-9 CAPLUS
CN Benzeneacetic acid, α-[(3,5-dimethoxyphenyl)methylene]-4-hydroxy-, methyl ester, (αE)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 606932-85-8 CAPLUS
CN Benzeneacetic acid, α-[(3,5-dimethoxyphenyl)methylene]-4-hydroxy-, methyl ester, (αZ)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



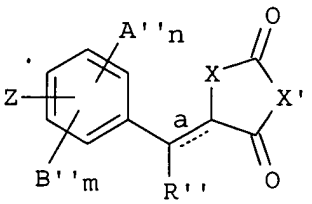
RE.CNT 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 4 OF 11 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2002:185699 CAPLUS
DN 136:247571
TI Preparation of novel heterocyclic analogs of diphenylethylene compounds as inhibitors of cytokines or cyclooxygenase
IN Nag, Bishwajit; Dey, Debendranath; Medicherla, Satyanarayana; Neogi, Partha

PA USA
SO U.S. Pat. Appl. Publ., 34 pp., Cont.-in-part of U.S. Ser. No. 785,554.
CODEN: USXXCO
DT Patent
LA English
FAN.CNT 9

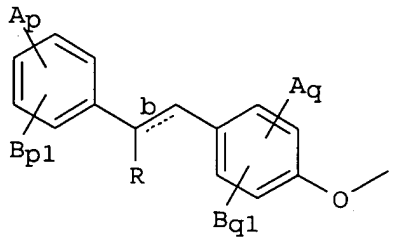
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 2002032225	A1	20020314	US 2001-843167	20010427
US 6245814	B1	20010612	US 1998-74925	19980508
US 2002025975	A1	20020228	US 2001-785554	20010220
CA 2410171	AA	20011220	CA 2001-2410171	20010605
WO 2001095859	A2	20011220	WO 2001-US17950	20010605
WO 2001095859	A3	20030828		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 2001066670	A5	20011224	AU 2001-66670	20010605
EP 1360178	A2	20031112	EP 2001-944241	20010605
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY, TR				
JP 2004527455	T2	20040909	JP 2002-510041	20010605
US 2003181494	A1	20030925	US 2002-265902	20021008
US 2004186299	A1	20040923	US 2004-808519	20040325
PRAI US 1998-74925	A2	19980508		
US 1999-287237	A2	19990406		
US 2000-591105	A2	20000609		
US 2001-785554	A2	20010220		
US 2001-843167	A	20010427		
WO 2001-US17950	W	20010605		

OS MARPAT 136:247571
GI

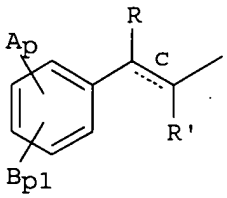


I

Q =



Q1 =

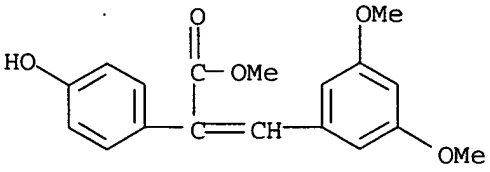


AB Novel diphenylethylene compds. and derivs. thereof containing thiazolidinedione or oxazolidinedione moieties are provided which are

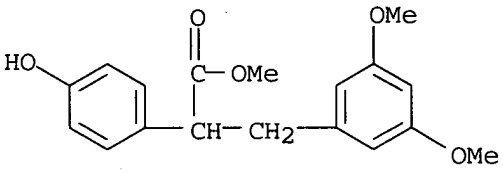
effective in lowering blood glucose level, serum insulin, triglyceride and free fatty acid levels in animal models of Type II diabetes. The above compds. and their derivs. are resented by formula [I; Z = Q, Q1, H, A", B"; wherein n, m, q, q1 = integers from zero to 4 provided that n+m≤4 and q+q1≤4; p, p1 = integers from zero to 5 provided that p+p1≤5; a, b and c are double bonds which may be present or absent; when present; the double bonds may be in the E or Z configuration and, when absent, the resulting stereocenters may have the R- or S-configuration; R, R', R" = H, C1-20 linear or branched alkyl, C2-20 linear or branched alkenyl, CO2Z' (wherein Z' = H, Na, K, or other pharmaceutically acceptable counterion such as Ca, Mg, ammonium, tromethamine, and the like), CO2R''', NH2, NHR''', N(R''')2, OH, OR''', halo, substituted C1-20 linear or branched alkyl or substituted C2-20 linear or branched alkenyl (wherein R''' is C1-20 linear or branched alkyl or linear or branched alkenyl); A, A', A'' = H, C1-20 acylamino, C1-20 acyloxy, C1-20 alkanoyl, C1-20 alkoxycarbonyl, C1-20 alkoxy, C1-20 alkylamino, C1-20 alkylcarboxylamino, CO2H, cyano, halo, HO; B, B', B'' = H, C1-20 acylamino, C1-20 acyloxy, C1-20 alkanoyl, C1-20 alkenoyl, C1-20 alkoxycarbonyl, C1-20 alkoxy, C1-20 alkylamino, C1-20 alkylcarboxylamino, aroyl, aralkanoyl, CO2H, cyano, halo, HO; or A and B together, or A' and B' together, or A'' and B'' together, may be joined to form a methylenedioxy or ethylenedioxy group; and X, X' are independently -NH, -NR''', O or S]. In contrast to previously reported thiazolidinedione compds., known to lower leptin levels, the present compds. increase leptin levels and have no known liver toxicity. They inhibit the activity of TNF-alpha, interleukin IL-1 or IL-6 or cyclooxygenase-2 (COX-2). The compds. are disclosed as useful for a variety of treatments including the treatment of inflammation, inflammatory and immunol. diseases, insulin resistance, hyperlipidemia, coronary artery disease, cancer and multiple sclerosis. Thus, To a mixture of 3,5-dimethoxybenzaldehyde (500 g) and p-hydroxyphenylacetic acid (457 g) was added acetic anhydride (1 L) and triethylamine (420 mL) and the nonhomogeneous mixture on heating became homogeneous at 70° and stirred at 130-140° for 6 h to give 47% 3-(3,5-dimethoxyphenyl)-2-(4-hydroxyphenyl)acrylic acid (II) (428 g). II (427.5 g) was suspended in 3 L methanol, treated with 100 mL concentrated H2SO4, and heated at reflux for 20 h under Ar to give 97% 3-(3,5-dimethoxyphenyl)-2-(4-hydroxyphenyl)acrylic acid Me ester (III). III (433 g) was dissolved in 1.6 L DMF, treated with 60.4 g NaH (50% in oil) and the with 185 mL p-fluorobenzaldehyde, and heated at 180° for 18 h to give 77% 3-(3,5-dimethoxyphenyl)-2-[4-(4-formylphenoxy)phenyl]acrylic acid Me ester which (352 g), 2,4-thiazolidinedione 98.6, benzoic acid 134, and piperidine 107.4 g were heated in 2.5 L toluene at reflux with continuous removal of H2O through Dean-Stark apparatus to give 86% 3-(3,5-dimethoxyphenyl)-2-[4-[4-(2,4-dioxothiazolidin-5-ylidenemethyl)phenoxy]phenyl]acrylic acid Me ester (IV). IV (30 g) was hydrogenated over 15 g 10% Pd-C in 900 mL dioxane in a Parr apparatus at 60 Psi for 24 h, followed by adding 15 g 10% Pd-C and continuing the hydrogenation for another 24 h to give 86% 3-(3,5-dimethoxyphenyl)-2-[4-[4-(2,4-dioxothiazolidin-5-ylmethyl)phenoxy]phenyl]acrylic acid Me ester (V). When V was orally administered to ob/ob mice with a single oral dose (50 mg/kg body weight), there was a 62 % drop in blood glucose level and, similar to db/db mice, there was no significant increase in body weight between the control and the treatment groups. This was in contrast to treatment of diabetic animals by thiazolidinedione type compds. which are known to be associated with increase in body weight

IT **380881-27-6P**, 3-(3,5-Dimethoxyphenyl)-2-(4-hydroxyphenyl)acrylic acid methyl ester
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of novel heterocyclic analogs of phenylethylene compds. as inhibitors of cytokines or cyclooxygenase for therapeutic agents)

RN 380881-27-6 CAPLUS
CN Benzeneacetic acid, α-[(3,5-dimethoxyphenyl)methylene]-4-hydroxy-, methyl ester (9CI) (CA INDEX NAME)



IT **380881-43-6P**, 3-(3,5-Dimethoxyphenyl)-2-(4-hydroxyphenyl)propionic acid methyl ester
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of novel heterocyclic analogs of phenylethylene compds. as inhibitors of cytokines or cyclooxygenase for therapeutic agents)
RN 380881-43-6 CAPLUS
CN Benzenepropanoic acid, α-(4-hydroxyphenyl)-3,5-dimethoxy-, methyl ester (9CI) (CA INDEX NAME)



L6 ANSWER 5 OF 11 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2002:158391 CAPLUS
DN 136:216745
TI Preparation and activity of diphenylethylene thiazolidinediones and analogs as antidiabetics, antiinflammatories, or immunomodulators
IN Nag, Bishwajit; Dey, Debendranath; Medicherla, Satyanarayana; Neogi, Partha
PA USA
SO U.S. Pat. Appl. Publ., 30 pp., Cont.-in-part of U.S. Ser. No. 591,105.
CODEN: USXXCO
DT Patent
LA English
FAN.CNT 9

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 2002025975	A1	20020228	US 2001-785554	20010220
US 6245814	B1	20010612	US 1998-74925	19980508
US 2002032225	A1	20020314	US 2001-843167	20010427
CA 2410171	AA	20011220	CA 2001-2410171	20010605
WO 2001095859	A2	20011220	WO 2001-US17950	20010605
WO 2001095859	A3	20030828		

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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR,

IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

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	EP 1360178	A2	20031112	EP 2001-944241	20010605
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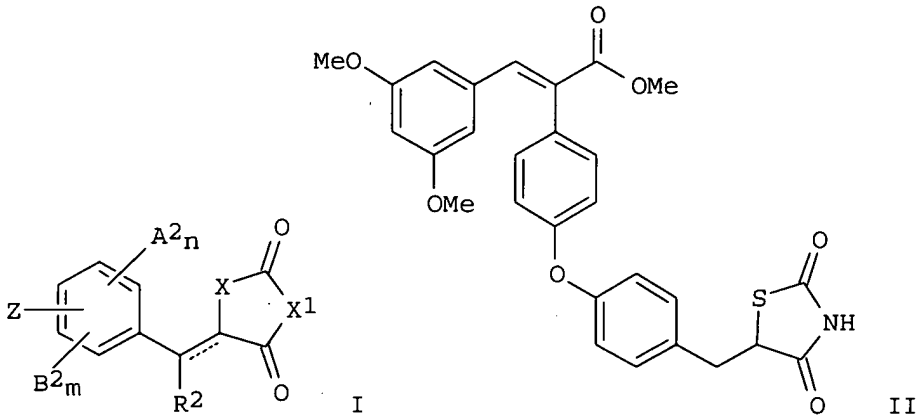
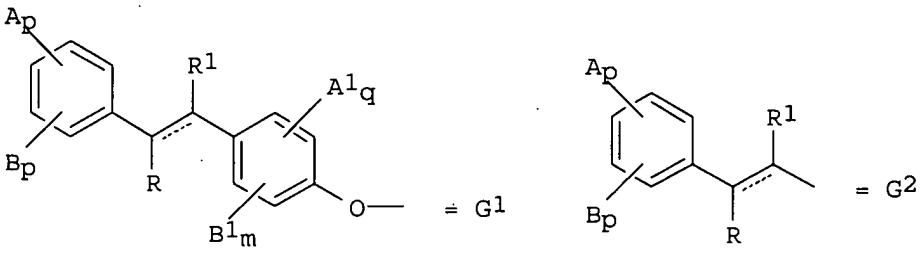
	US 2003181494	A1	20030925	US 2002-265902	20021008
	US 2004186299	A1	20040923	US 2004-808519	20040325
PRAI	US 1998-74925	A2	19980508		
	US 1999-287237	A2	19990406		
	US 2000-591105	A2	20000609		
	US 2001-785554	A2	20010220		
	US 2001-843167	A	20010427		
	WO 2001-US17950	W	20010605		

OS MARPAT 136:216745

GI





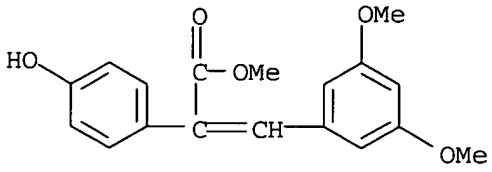
AB Title compds. I [wherein Z = G1, H, A2, B2, or G2; n, m, and q = independently 0-4; p = independently 0-5; R, R1, and R2 = independently H, (un)substituted alkyl or alkenyl, CO2Z1, CO2R3, NH2, NHR3, NR32, OH, OR3, or halo; Z1 = H, Na, K, or other pharmaceutically acceptable counterion; R3 = alkyl or alkenyl; A, A1, and A2 = independently H, acylamino, acyloxy, alkanoyl, alkoxycarbonyl, alkoxy, alkylamino, alkylcarboxylamino, carboxyl, CN, H, or OH; B, B1, and B2 = independently H, acylamino, acyloxy, alkanoyl, alkenoyl, alkoxycarbonyl, alkoxy, alkylamino, alkylcarboxylamino, aroyl, aralkanoyl, carboxyl, CN, halo, or OH; or A and B or A1 and B1 or A2 and B2 together form a methylenedioxy or ethylenedioxy group; X and X1 = independently NH, NR3, O, or S] are provided which are effective in lowering blood glucose level, serum insulin, triglyceride, and free fatty acid levels in animal models of Type II diabetes. In contrast to previously reported thiazolidinedione

compds., known to lower leptin levels, the present compds. increase leptin levels and have no known liver toxicity. Thus, II was prepared in five steps by condensation of 3,5-dimethoxybenzaldehyde with 4-hydroxyphenylacetic acid (47%), followed by esterification (97%), etherification with 4-fluorobenzaldehyde (77%), condensation with 2,4-thiazolidinedione (86%), and hydrogenation of the ylidene double bond (40%). Oral administration of II to obese mice caused a 62% drop in blood glucose level. I are useful for the treatment of inflammation, inflammatory and immunol. diseases, insulin resistance, hyperlipidemia, coronary artery disease, cancer, and multiple sclerosis.

IT **380881-27-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and activity of diphenylethylene thiazolidinediones and analogs as antidiabetics, antiinflammatories, or immunomodulators)

RN 380881-27-6 CAPLUS

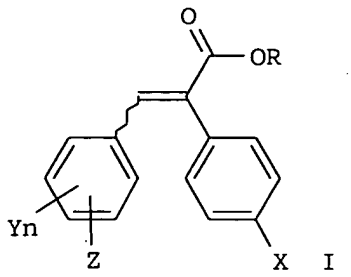
CN Benzeneacetic acid, α-[(3,5-dimethoxyphenyl)methylene]-4-hydroxy-, methyl ester (9CI) (CA INDEX NAME)



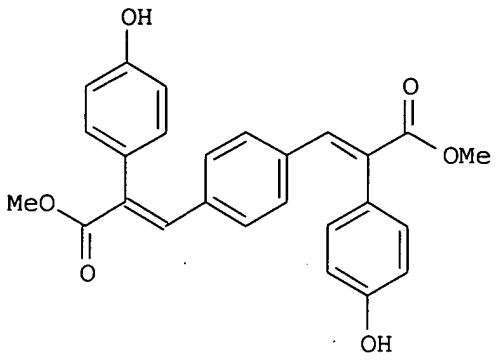
L6 ANSWER 6 OF 11 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2002:31392 CAPLUS
DN 136:85656
TI Alpha-arylated cinnamic esters and 1,4-bis(α-carboxyl-β-styryl)benzene esters as uv-blocking agents
IN Lakner, Frederick J.; Nag, Bishwajit; Neogi, Partha
PA Calyx Therapeutics, Inc., USA
SO PCT Int. Appl., 16 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002002501	A1	20020110	WO 2001-US20013	20010622
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	US 6413504	B1	20020702	US 2000-610098	20000630
PRAI	US 2000-610098	A	20000630		

OS MARPAT 136:85656
GI



I



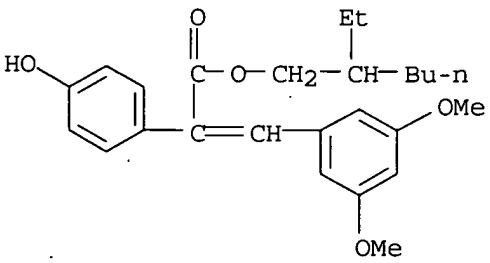
II

AB Compds. of formula I [R = H, C1-C20 alkyl, or C5-C20 aryl; Z, X, Y = independently H, acylamino, acyloxy, alkoxycarbonyl, amino, C1-C20 alkyl, alkoxy, hydroxy, alkylamino, etc.; n = 1-4] were prepared and their molar extinction coeffs. at 305 nm (UVB radiation) and 350 nm (UVA radiation) were calculated and compared to com. sunscreening agents. Thus, II was produced via the Perkin condensation of terephthaldicarboxaldehyde with p-hydroxyphenyl acetic acid followed by esterification with methanol in sulfuric acid.

IT **387354-16-7P**
RL: COS (Cosmetic use); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(alpha-arylated cinnamic esters and 1,4-bis(alpha-carboxyl-beta-styryl)benzene esters as uv-blocking agents)

RN 387354-16-7 CAPLUS

CN Benzeneacetic acid, α-[(3,5-dimethoxyphenyl)methylene]-4-hydroxy-, 2-ethylhexyl ester (9CI) (CA INDEX NAME)



RE.CNT 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 7 OF 11 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2001:923567 CAPLUS
DN 136:37596

TI Preparation and activity of diphenylethylene thiazolidinedione or oxazolidinedione compounds as antidiabetics or antiinflammatories

IN Neogi, Partha; Nag, Bishwajit; Medicherla, Satyanarayana; Dey, Debendranath

PA Calyx Therapeutics, Inc., USA

SO PCT Int. Appl., 76 pp.
CODEN: PIXXD2

DT Patent

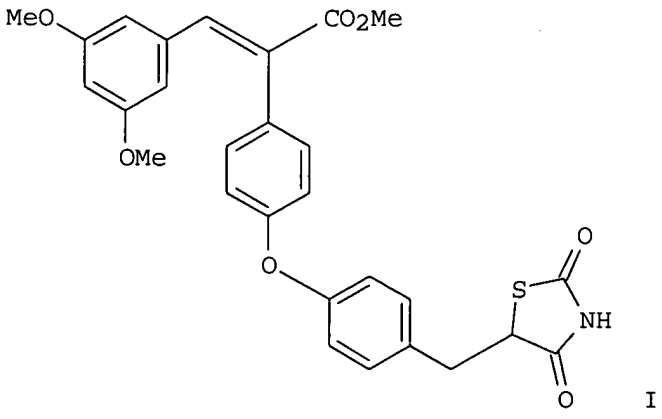
LA English

FAN.CNT 9

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001095859	A2	20011220	WO 2001-US17950	20010605
	WO 2001095859	A3	20030828		
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	US 2002025975	A1	20020228	US 2001-785554	20010220
	US 2002032225	A1	20020314	US 2001-843167	20010427
	CA 2410171	AA	20011220	CA 2001-2410171	20010605
	AU 2001066670	A5	20011224	AU 2001-66670	20010605
	EP 1360178	A2	20031112	EP 2001-944241	20010605
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY, TR				
	JP 2004527455	T2	20040909	JP 2002-510041	20010605
PRAI	US 2000-591105	A2	20000609		
	US 2001-785554	A2	20010220		
	US 2001-843167	A2	20010427		
	US 1998-74925	A2	19980508		
	US 1999-287237	A2	19990406		
	WO 2001-US17950	W	20010605		

OS MARPAT 136:37596

GI



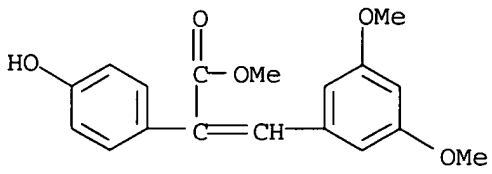
I

AB Novel diphenylethylene compds. and derivs. thereof containing thiazolidinedione or oxazolidinedione moieties are provided which are effective in lowering blood glucose level, serum insulin, triglyceride and free fatty acid levels in animal models of Type II diabetes. In contrast

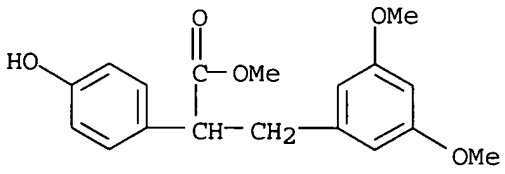
to previously reported thiazolidinedione compds., known to lower leptin levels, the present compds. increase leptin levels and have no known liver toxicity. Thus, (I) was prepared in five steps by condensation of 3,5-dimethoxybenzaldehyde with 4-hydroxyphenylacetic acid followed by esterification and etherification with 4-fluorobenzaldehyde and condensation with 2,4-thiazolidinedione and hydrogenation of the ylidene double bond. Oral administration of I to obese mice caused a 62% drop in blood glucose level. The compds. are disclosed as useful for a variety of treatments including the treatment of inflammation, inflammatory and immunol. diseases, insulin resistance, hyperlipidemia, coronary artery disease, cancer and multiple sclerosis.

IT **380881-27-6P 380881-43-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and activity of diphenylethylene thiazolidinedione or oxazolidinedione compds. as antidiabetics or antiinflammatories)

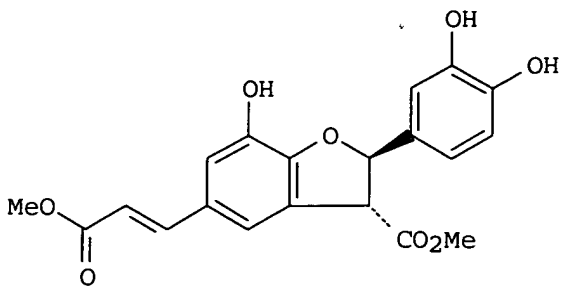
RN 380881-27-6 CAPLUS
CN Benzeneacetic acid, α-[(3,5-dimethoxyphenyl)methylene]-4-hydroxy-, methyl ester (9CI) (CA INDEX NAME)



RN 380881-43-6 CAPLUS
CN Benzenepropanoic acid, α-(4-hydroxyphenyl)-3,5-dimethoxy-, methyl ester (9CI) (CA INDEX NAME)



L6 ANSWER 8 OF 11 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1999:771171 CAPLUS
DN 132:122418
TI Synthesis and biological evaluation of dihydrobenzofuran lignans and related compounds as potential antitumor agents that inhibit tubulin polymerization
AU Pieters, Luc; Van Dyck, Stefaan; Gao, Mei; Bai, Ruoli; Hamel, Ernest; Vlietinck, Arnold; Lemiere, Guy
CS Department of Pharmaceutical Sciences, University of Antwerp, Belgium, B-2610, Belg.
SO Journal of Medicinal Chemistry (1999), 42(26), 5475-5481
CODEN: JMCMAR; ISSN: 0022-2623
PB American Chemical Society
DT Journal
LA English
GI



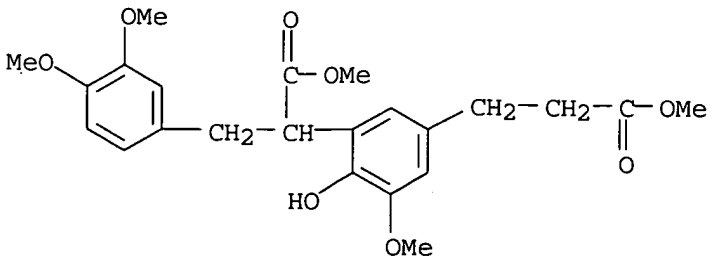
I

AB A series of 19 related dihydrobenzofuran lignans and benzofurans was obtained by a biomimetic reaction sequence involving oxidative dimerization of p-coumaric, caffeic, or ferulic acid Me esters, followed by derivatization reactions. All compds. were evaluated for potential anticancer activity in an in vitro human disease-oriented tumor cell line screening panel that consisted of 60 human tumor cell lines arranged in nine subpanels, representing diverse histologies. Leukemia and breast cancer cell lines were relatively more sensitive to these agents than were the other cell lines. Me (E)-3-[2-(3,4-dihydroxyphenyl)-7-hydroxy-3-methoxycarbonyl-2,3-dihydro-1-benzofuran-5-yl]prop-2-enoate (I), the dimerization product of caffeic acid Me ester, containing a 3',4'-dihydroxyphenyl moiety and a hydroxyl group in position 7 of the dihydrobenzofuran ring, showed promising activity. The average GI50 value (the molar drug concentration required for 50% growth inhibition) of I was 0.3 μM. Against three breast cancer cell lines, I had a GI50 value of <10 nM. Methylation, reduction of the double bond of the C3-side chain, reduction of the methoxycarbonyl functionalities to primary alcs., or oxidation of the dihydrobenzofuran ring to a benzofuran system resulted in a decrease or loss of cytotoxic activity. Compound I inhibited mitosis at micromolar concns. in cell culture through a relatively weak interaction at the colchicine binding site of tubulin. In vitro it inhibited tubulin polymerization by 50% at a concentration of 13 ± 1 μM. The 2R,3R-enantiomer of I was twice as active as the racemic mixture, while the 2S,3S-enantiomer had minimal activity as an inhibitor of tubulin polymerization These dihydrobenzofuran lignans (2-phenyl-dihydrobenzofuran derivs.) constitute a new group of antimitotic and potential antitumor agents that inhibit tubulin polymerization

IT **256330-13-9P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis and biol. evaluation of dihydrobenzofuran lignans and related compds. as potential antitumor agents that inhibit tubulin polymerization)

RN 256330-13-9 CAPLUS

CN Benzenepropanoic acid, α-[2-hydroxy-3-methoxy-5-(3-methoxy-3-oxopropyl)phenyl]-3,4-dimethoxy-, methyl ester (9CI) (CA INDEX NAME)



RE.CNT 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 9 OF 11 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1980:6338 CAPLUS
DN 92:6338
TI Total synthesis of heptamethyl lithospermate
AU Jacobson, Richard M.; Raths, Richard A.
CS Dep. Chem., Indiana Univ., Bloomington, IN, 47405, USA
SO Journal of Organic Chemistry (1979), 44(22), 4013-14
CODEN: JOCEAH; ISSN: 0022-3263
DT Journal
LA English
GI

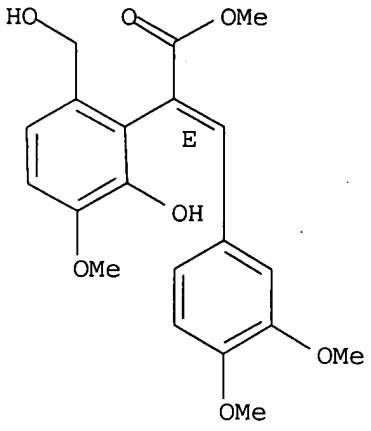
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB 2-Allylisovanillin was reduced with NaBH4, acetylated with Ac2O, ozonized, and oxidized with H2CrO4 to give 2-acetoxy-6-(acetoxymethyl)-3-methoxybenzeneacetic acid, which was saponified and lactonized (Ac2O) to give benzopyranone I. Condensation of I with veratral followed by methanolysis of the lactone and oxidation of the resulting benzyl alc. with (COCl)2/Me2SO gave aldehyde II. Cyclization of II with HBr gave trans-dihydrobenzofuran III. Doebner condensation of III with malonic acid followed by esterification with Me 3,4-dimethoxyphenyllactate gave heptamethyl lithospermate (IV).

IT **71734-07-1P 71734-08-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediate in total synthesis of heptamethyl lithospermate)

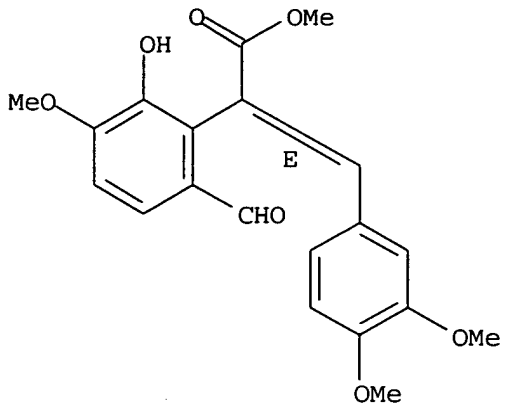
RN 71734-07-1 CAPLUS
CN Benzeneacetic acid, α-[(3,4-dimethoxyphenyl)methylene]-2-hydroxy-6-(hydroxymethyl)-3-methoxy-, methyl ester, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 71734-08-2 CAPLUS
CN Benzeneacetic acid, α-[(3,4-dimethoxyphenyl)methylene]-6-formyl-2-hydroxy-3-methoxy-, methyl ester, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L6 ANSWER 10 OF 11 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1963:486261 CAPLUS
DN 59:86261
OREF 59:5096b-h,5097a-e
TI Wilting agents and antibiotics. XXVIII Synthesis of 2,4 dimethoxy 6 hydroxyphenanthrene and constitution of orchinol.
AU Hardegger, E.; Biland, H. R.; Corrodi, H.
CS Eidg. Tech. Hochschule, Zuerich, Switz.
SO Helv. Chim. Acta (1963), 46, 1354-60
DT Journal
LA German
GI For diagram(s), see printed CA Issue.
AB (All m.ps. are corrected). 3,5 (MeO)2C6H3CH2CN [prepared from tech. α-resorcylic acid via 3,5-(MeO)2C6H3CO2H] (160 g.) refluxed 16 h. with 1.6 l. 20% aqueous KOH and the solution cooled, filtered, extracted with a little Et2O, and acidified with concentrated HCl gave 160 g. 3,5-(MeO)2C6H3CH2CO2H (I), m. 100-1°. I (30 g.) and 30 g. 2,4(O2N)2C6H3CHO dissolved in 300 mL. Ac2O, the solution treated with 21.5 mL. Et3N (the temperature rose to 40-50°), kept 16 h., concentrated in vacuo (H2O pump) at 50-60° to 50-75 mL., treated with 75 mL. H2O at 90° with vigorous shaking, the precipitate filtered off, washed with H2O, dried in vacuo, boiled with 100 mL. C6H6, filtered off while hot, and dried gave 37 g. 2,4 (O2N)2C6H3CH: C[C6H3(OMe)2-3,5]CO2R (II) (R = H), m. 205-6° (C6H6). II (R = H) (3.75 g.) suspended in 200 mL. Et2O treated with Et2OCH2N2 until all solid dissolved and N evolution ceased, the solution evaporated, the residue chromatographed on Al2O3 (activity II), and the product eluted with C6H6 gave 3.9 g. II (R = Me), needles, m. 95-6° (Et2O-MeOH); sometimes II (R = Me) was obtained as rhombohedrons, m. 118°; seeding an Et2O solution of the low melting ester with crystals of the higher melting ester gave quant. higher melting ester. II (R = Me) (3.88 g.) in 200 mL. MeOH hydrogenated over 500 mg. 10% Pd-C (after 1 h. and 22 h. 1600 mL. H and 1710 mL. H, resp., was absorbed), the solution filtered, evaporated in vacuo, and the residual oil (3.3 g.) treated with MeOH gave α-(3,5 dimethoxyphenyl)-β-(2,4 diaminophenyl)propionic acid δ-lactam, m. 185° (CHCl3-MeOH); Ac derivative m. 256-8° (CHCl3-MeOH). II (R = H) (10 g.) dissolved in 150 mL. hot AcOH, the solution treated with 18.2 g. SnCl2.2H2O in 30 mL. AcOH at 20° with stirring, saturated with HCl at 0°, stirred 24 h., concentrated in vacuo at 40° to 30 mL., dissolved in 200 mL. Et2O, the solution washed with 7 50-mL. portions H2O until the wash H2O was colorless, extracted with 3 50-mL. portions 2N NaOH, the combined exts. acidified with concentrated HCl, the product isolated with CH2Cl2, dissolved in 50 mL. EtOH, and the solution treated with HCl, the product, α-(3,5 dimethoxyphenyl) 2 amino 4 nitrocinnamic acid HCl salt (III.HCl), m.

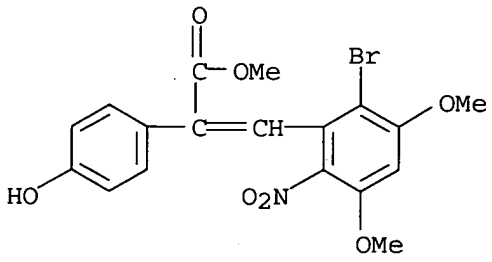
70° (decomposition), filtered off, treated with 150 mL. 1:1 EtOH-H2O, the mixture boiled until a clear solution formed, and the solution concentrated to 75 mL. and cooled gave 2.7 g. III, m. 205° (CHCl3-MeOH). III treated with CH2N2 in Et2O, the product chromatographed on Al2O3 (activity II), and the column eluted with CH2Cl2 and Et2O gave Me ester of III, m. 172° (MeOH-CHCl8). III (2.4 g.) dissolved in 36 mL. concentrated H2SO4 at -10°, the solution poured on 130 g. ice, treated during 15 min. with 1.45 mL. 5N NaNO2 at 0° with stirring, stirred 1.5 h., treated with 100 mL. H2O, stirred 1.5 h., treated with a small amount of urea (after 0.5 h. HNO2 was no longer detectable with KI-starch paper), filtered through Celite, the filter cake washed with H2O until no reaction with β-naphthol was obtained, the combined filtrates concentrated by boiling 45 min. at 100°, the precipitate filtered off, esterified with CH2N2, the product chromatographed on Al2O3 (activity II), and the column eluted with C6H6 gave 1.13 g. 2,4 dimethoxy 6 nitro 10 phenanthrenecarboxylic acid (IV) Me ester (V), m. 198° (C6H6). V (20 mg.) in 10 mL. MeOH boiled 2 h. with 2 mL. N KOH, diluted with 20 mL. H2O, and acidified with a few drops concentrated HCl gave IV, m. 280-1° (decomposition) (CH2Cl2-MeOH). V (1.04 g.) in 125 mL. THF hydrogenated over 1 g. prereduced 10% Pd-C (after 10 min. 190 mL. H absorbed, after 3 h. 207 mL. H, and finally 228 mL. H after 1 min. after addition of 500 mg. prereduced 10% Pd-C) gave 6-NH2 analog (VI) of V, m. 147-8° (MeOH). VI (622 mg.) dissolved in 20 mL. concentrated H2SO4 at -10°, the solution poured on 100 g. ice with shaking, the resulting suspension treated during 16 min. with 2.1 rel. N NaNO2 at 0°, the mixture stirred 2 h. at 0°, diluted with 100 mL. H2O, stirred 2 h., treated with urea, stirred 0.5 h. (excess HNO2 was now destroyed), heated 0.5 h. at 100°, cooled, the precipitate (650 mg.) filtered off, boiled 3 h. with 20 mL. MeOH and 5 mL. H2O containing 1 g. KOH, the solution evaporated, the residue dissolved in 20 mL. H2O, the solution acidified with concentrated HCl, the precipitate filtered off, decarboxylated by boiling 2.5 h. in 10 mL. quinoline with 100 mg. Cu chromite, the mixture added to 100 mL. 2N HCl, filtered, the filter cake and filtrate extracted with Et2O, the combined exts. evaporated, the residual oil (235 mg.) chromatographed on Al2O3 (activity II), the column cluted with C6H6-Et2O, and the product (63 mg.) crystallized from C6H6-hexane gave 8 mg. 2,4-dimethoxy-6hydroxyphenanthrene (VII), m. 135°. VI (311 mg.) diazotized and the solution of diazonium salt boiled down as above, the precipitate (350 mg.) filtered off, treated in 100 mL. MeOH with excess Et2O-CH2N2, after cessation of N evolution the solution evaporated, the residual oil (378 mg.) chromatographed on Al2O3 (activity II), and the product eluted with C6H6 gave 54 mg. Me 2,4,6-trimethoxy-10-phenanthrenecarboxylate, m. 130-1°, which was saponified and decarboxylated as above and then chromatographed on Al2O3 (activity II) and eluted with C6H6 to give 17 mg. 2,4,6trimethoxyphenanthrene (VIII), m. 109-10° (hexane). Dehydroorchinol (m. 168-70°) was different from synthetic VIII (m. 136°). Although the m.ps. of dehydroorchinol Me ether (m. 113-14°) and synthetic VIII (m. 109-10°) differed only slightly, the mixed m.p. was depressed by 25-30°. From this, it followed that orchinol (Villa) was 2,4-dimethoxy-7-hydroxy-9,10-dihydrophenanthrene. As a supplement to the synthesis of VII was mentioned another route (see below) which, although not carried to completion, should also lead to VII. 2,3,5, 6-Br(MeO)2(O2N) C6HCHO (29 g.) dissolved in 900 mL. hot Ac2O, the solution treated with 30.5 g. p-HOC6H4CH2CO2H and 14 mL. Et3M at 20°, kept 6 h. at 95-100° with periodic shaking, concentrated in vacuo to 50 mL., heated to 90° with 50 mL. H2O, evaporated in vacuo, the residual solid dried 6 h. in vacuo, heated to boiling with 150 mL. C6H6, and the solution filtered and evaporated gave 20.2 g. 2,3,5,6-Br(MeO)2(O2N)C6HCH:C(C6H4OR-4)CO2R' (IX) (R = R' = H) (X), m. 263-6° (slight decomposition above 230°) (dioxane). X (3 g.) suspended in 200 mL. MeOH treated with

Et2O-CH2N2 (all solid dissolved) gave IX (R = H, R' = Me), m. 210-11° (MeOH) X (4.3 g.) in a little H2O treated portionwise during 1 h. with 18 mL. 4N KOH and 3.8 g. Me2SO4 at 100° with stirring in such a way that the mixture always remained alkaline, the whole stirred 0.5 h. at 100°, diluted with H2O, filtered, and the filtrate acidified with. 2N HCl gave 3.5 g. IX (R = Me, R' = H), m. 224° (EtOHCCl4). X (3.47 g.) in 100 mL. EtOH refluxed 21 h. with 3 g. K2CO3 and 2.5 mL. PhCH2Cl, the solution filtered, evaporated, the residue dissolved in
300 mL. N Na2CO3, the solution washed with Et2O, brought to pH 1-2 with concentrated HCl, and the product isolated with CHCl3 gave 1.8 g. IX (R = PhCH2, R' = H), m. 2357° (CHCl3-MeOH), which was treated in 1:1 MeOH-Me2CO with Et2O-CH2N2 to give IX (R = PhCH2, R' = Me), m. 187° (Et2O-petr. ether).

IT **93870-75-8**, Acrylic acid, 3-(2-bromo-3,5-dimethoxy-6-nitrophenyl)-2-(p-hydroxyphenyl)-, methyl ester
(preparation of)

RN 93870-75-8 CAPLUS

CN Acrylic acid, 3-(2-bromo-3,5-dimethoxy-6-nitrophenyl)-2-(p-hydroxyphenyl)-, methyl ester (7CI) (CA INDEX NAME)



L6 ANSWER 11 OF 11 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1963:428381 CAPLUS

DN 59:28381

OREF 59:5094g-h,5095a-h,5096a-b

TI Wilting agents and antibiotics. XXVII. Induced defensive substances in the Orchidaceae. 2

AU Hardegger, E.; Schellenbaum, M.; Corrodi, H.

CS Eidg. Tech. Hochschule, Zuerich, Switz.

SO Helvetica Chimica Acta (1963), 46, 1171-80
CODEN: HCACAV; ISSN: 0018-019X

DT Journal

LA German

GI For diagram(s), see printed CA Issue.

AB Biol. investigations have shown that under the influence of certain morbific agents, defensive substances are produced in the corms of Orchidaceae; e.g., the mycorrhizal fungus Rhizoctonia repens activates defense mech anisms in the corms of Orchis militaris, which clearly result in the formation of orchinol (I), C16H16O3, as the sole defensive substance, along with biol. inactive p-HOC6H4CH2OH (II); both I and II are not found in healthy plants. However, Loroglossum hircinum produces no I, but other defensive substances against R. repens. From infected corms of L. hircinum was isolated a biol. inactive compound, C16H16O3, designated lorroglossol (III), isomeric with and closely related to I. (All m.ps. are corrected). The Et2Oeluate (loc. cit.) chromatographed again on Al2O3 (activity II) gave II, m. 120° (MeOH-H2O), mol. weight (camphor) 136. pHOC6H4CO2Me (10 g.) in 150 mL. Et2O added dropwise to 6 g. LiAlH4 in 100 mL. Et2O at 20° with stirring, the whole refluxed 3 h., decomposed with EtOAc and H2O under ice cooling, acidified with AcOH, and the product isolated with Et2O gave 2 g. II, m. 122° (H2O). I (20

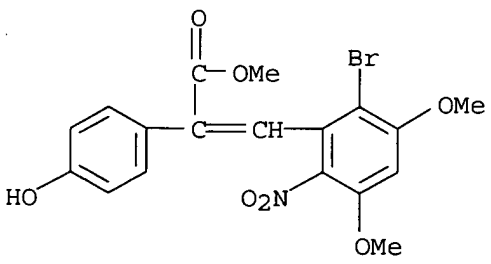
γ) in 20 μl. MeOH applied to Whatman Number 1 paper, the solution allowed to travel with 1:1 MeOH-H2O, the paper dried, sprayed with 0.1% alc. N,2,6 trichloro-ρ-benzoquinone imine, followed by saturated aqueous borax, and dried gave a grayish green spot corresponding to I with Rf 0.56; I had Rf 0.79 with 1:1 EtOH-H2O. EtOH-Et2O-exts. of infected corm fragments of L. hircinum were prepared and worked up in a manner similar to the isolation of I from the corms of O. militaris to give III, m. 98° (C6H6cyclohexane, then MeOH). III (50 mg.), 0.1 mL. Me2SO4, and 140 mg. K2CO3 in 10 mL. Me2CO refluxed 22 h., cooled, filtered, the filtrate evaporated, the residue (52 mg.) chromatographed on Al2O3 (activity I), and the column eluted with CH2Cl2 gave 27 mg. Me ether of III, b0.1 200°. I (20 mg.) and 93 mg. 3,5(O2N)2C6H3COCl in 1 mL. absolute pyridine kept 30 min. at 20°, boiled 2 min., cooled, diluted with 20 mL. Et2O, filtered, the filtrate washed with dilute HCl, saturated aqueous KHCO3, and saturated salt solution, dried, and evaporated gave 30 mg. I 3,5 dinitrobenzoate, m. 198° (CH2Cl-Et2O). A solution of 500 mg. I, 1.9 g. ρ-MeC6H4SO2Cl (IIIa), and 5 mL. pyridine was prepared at 0°, kept 24 h. at 20°, treated with 1 mL. H2O, kept 1 h., taken up in CHCl3, and the solution washed (dilute HCl, saturated aqueous KHCO3, and H2O) and evaporated to give 774 mg. I tosylate (IV), oil which crystallized, m. 101-3° (MeOH-H2O). IV (50 mg.) and 25 mg. NaI in Me2CO or in Ac2O refluxed 5 h. gave (from each experiment) quant. unchanged IV. IV (100 mg.) and 100 mg. LiAlH4 in 5 mL. dioxane refluxed 2 h., treated with EtOAc and H2O to destroy excess LiAlH4, acidified with AcOH, and the product isolated with Et2O (the extract was washed in the usual manner) gave 59 mg. I after crystallization from C6H6-cyclohexane. Saponification of IV with dilute aqueous NaOH also gave I. I (300 mg.) in 6 mL. Et2O and 21 mL. 2% Et2O-CH2N2 kept 12 h. at 20°, the solution filtered, evaporated, the residue chromatographed on Al2O3 (activity II), and the column eluted with C6H6 gave 51 mg. Me ether (V) of I, m. 86-7° (cyclohexane); continued elution with 1:1 C6H6-Et2O gave 213 mg. unchanged I. I (340 mg.) stirred to a paste with a little H2O, the paste treated during 1 h. with alternate portions of 2.3 mL. 4N KOH (total) and 0.37 mL. Me2SO4 (total) at 100° in such a way that the mixture always remained alkaline, kept 30 min. at 100°, cooled, filtered, the filtrate extracted with C6H6, the extract washed, evaporated, and the residue purified as above gave 298 mg. V, m. 86-7°. To 128 mg. I in 2 mL. AcOH was added dropwise 80 mg. Br in 1 mL. AcOH and the solution poured into H2O to give di-Br derivative of I, m. 154° (CCl4). To 200 mg. I in 4 mL. CHCl3 and 10 mL. CCl4 was added dropwise during 30 min. 9 mL. 0.18 M CCl4-Br at 0°, the solution stirred 30 min. (no more free Cl was present) evaporated in vacuo, the residue (265 mg.) adsorbed on silica gel, the chromatogram developed with C6H6CHCl3, the column extruded, and the visible zones sectioned and eluted with CHCl3 to give 153 mg. di-Cl derivative of I, m. 133-40° (unsharp) (C6H6-cyclohexane, then sublimation in vacuo), and 63 mg. tri-Cl derivative of I, m. 198-9° (C6H6-cyclohexane, then sublimation in vacuo); the former compound migrated slower than the latter compound IV (750 mg.) in 60 mL. EtOH hydrogenated at atmospheric pressure over 4 g. fresh prereduced Raney Ni W-2, the hydrogenation continued (2 addns. of 2 g. fresh catalyst were made) (after 3 days 128 mL. H was absorbed), the solution filtered, evaporated, the partially crystalline residue dissolved in C6H6, the solution washed with H2O, evaporated, the residue (286 mg.) chromatographed on Al2O3 (activity I), and the column eluted with C6H6 gave 1st 58 mg. oil and then 228 mg. deoxyorchinol (VI), C16H16O2, m. 58-9° (pentane). VI (170 mg.) and 510 mg. pyridine-HCl heated 6 h. at 210-20°, the mixture partitioned between Et2O-2N HCl, and the

Et2O-layer washed (H2O and 2N NaOH) and evaporated gave 11 mg. neutral oily fraction; the NaOH-soluble product (135 mg.) chromatographed on silica gel and the product eluted with Et2O gave 117 mg. deoxydidemethylorchinol (VII), m. 145° (C6H6). o- (VIII) and pC6H4(OH)2 (IX) and VII (5 mg. each) in absolute Et2O and in absolute C6H6 were boiled 5 min. with 500 mg. Ag2O and kept overnight. VIII and IX gave instantaneous red and yellow colors, resp., with Et2O (even at 20°). VII did not give these color reactions. VII (100 mg.) and 0.2 mL. Ac2O in 1 mL. pyridine kept 12 h. at 20° and poured into ice H2O gave 117 mg. VII diacetate, m. 92-3° (C6H6-petr. ether). VII (75 mg.) and 665 mg. IIIa in 2 mL. pyri- dine kept 12 h. at 20° and worked up as was iV gave 173 mg. VII ditosylate, m. 163° (C6H6-Et2O). I (500 mg.) and 75 mg. 10% Pd-C heated 5 min. at 180-200° (34 mL. H obtained), the product chromatographed on Al2O3 (activity II), and the column eluted with 1:1 C6H6-Et2O gave 266 mg. dehydroorchinol (X), C16H14O3, m. 168-70° (C6H6). X (100 mg.) methylated with 0.11 mL. Me2SO4 and 0.7 mL. 4N KOH as above, the product chromatographed on Al2O3 (activity II), and the column eluted with 1:1 C6H6-petr. ether gave 94 mg. X Me ether (XI), m. 113-14°. V (540 mg.) and 80 mg. 10% Pd-C heated 5 h. at 210-80° (31 mL. H obtained), the product chromatographed on Al2O3 (activity II), eluted with C6H6-petr. ether, and recrystd. from C6H6-petr. ether gave 340 mg. XI, m. 111-13°; unchanged V remained in the mother liquor. VII (250 mg.) and 40 mg. 10% Pd-C heated 5 h. at 250-300° (6 mL. H and an undetd, amount H2O obtained), the petr. ethersol. fraction of the dehydrogenation product chromatographed on Al2O3 (activity I), and the column eluted with petr. ether gave 54 mg. phenanthrene, m. 94-5° (EtOH) [trinitrobenzene complex m. 158° (EtOH)]; the petr. ether insol. fraction recrystd. from C6H6-petr. ether gave 2 phenanthrol, m. 163-4° [acetate m. 139-40° (C6H6-petr. ether)]. VI (300 mg.) and 45 mg. 10% Pd-C heated 1 h. at 260-80° (21 mL. H obtained), the C6H6-soluble fraction of the dehydrogenation product chromatographed on Al2O3 (activity I), and the product eluted with 1:1 C6H6-petr. ether and repeatedly recrystd. from cyclohexane gave 146 mg. deoxydehydroorchinol (XII), C16H14O2, m. 75-6°, identical (mixed m.p. and UV and IR spectra) with 2,4 dimethoxyphenanthrene. XII (107 mg.) and 320 mg. pyridine-HCl heated 6 h. at 210-20°, the product (CHCl3-soluble, H2O-insol.) extracted with 2N NaOH, the extract acidified, the resulting oil (77 mg.) acetylated with Ac2O in pyridine, and this product chromatographed in silica gel and eluted with Et2O gave 52 mg. di O acetyldeoxydehydrodidemethylorchinol (XIII), m. 128-30°. These results indicated that I was either 2,4 dimethoxy 6 or 7 hydroxy 9,10 dihydrophenanthrene (XIV). The UV spectrum (EtOH) of I and the IR spectra (KBr) of I and XII were recorded.

IT **93870-75-8**, Acrylic acid, 3-(2-bromo-3,5-dimethoxy-6-nitrophenyl)-2-(p-hydroxyphenyl)-, methyl ester
(preparation of)

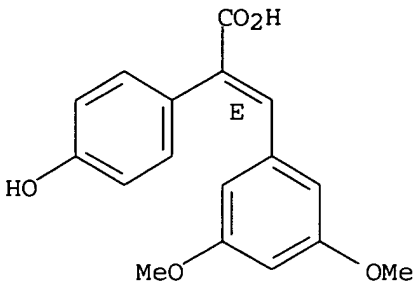
RN 93870-75-8 CAPLUS

CN Acrylic acid, 3-(2-bromo-3,5-dimethoxy-6-nitrophenyl)-2-(p-hydroxyphenyl)-, methyl ester (7CI) (CA INDEX NAME)



L2 ANSWER 6 OF 10 REGISTRY COPYRIGHT 2005 ACS on STN

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

CN Benzeneacetic acid, α-[(3,5-dimethoxyphenyl)methylene]-4-hydroxy-, (αE)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Benzeneacetic acid, α-[(3,5-dimethoxyphenyl)methylene]-4-hydroxy-, (E)-

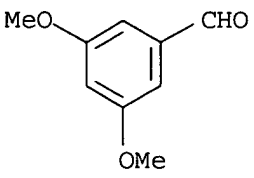
L2 ANSWER 7 OF 10 REGISTRY COPYRIGHT 2005 ACS on STN

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

CN Insulin (9CI) (CA INDEX NAME)
OTHER NAMES:
CN Actrapid
CN Actrapid HM
CN Actrapid MC
CN Decurvon
CN Dermulin
CN Endopancrine
CN Exubera
CN HMR 4006
CN Iletin
CN Insular
CN Insulin Injection
CN Insulyl
CN Intesulin B
CN Iszilin
CN Mixtard
CN Musulin

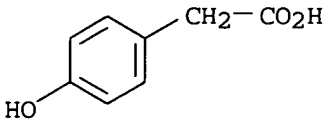
L2 ANSWER 8 OF 10 REGISTRY COPYRIGHT 2005 ACS on STN



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

CN Benzaldehyde, 3,5-dimethoxy- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)
OTHER NAMES:
CN 3,5-Dimethoxybenzaldehyde
CN NSC 62667

L2 ANSWER 9 OF 10 REGISTRY COPYRIGHT 2005 ACS on STN

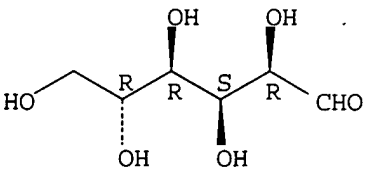


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

CN Benzeneacetic acid, 4-hydroxy- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Acetic acid, (p-hydroxyphenyl)- (8CI)
OTHER NAMES:
CN (4-Hydroxyphenyl)acetic acid
CN (p-Hydroxyphenyl)acetic acid
CN 2-[4-(Hydroxy)phenyl]acetic acid
CN 4-(Carboxymethyl)phenol
CN 4-Hydroxybenzeneacetic acid
CN NSC 25066
CN NSC 27460

L2 ANSWER 10 OF 10 REGISTRY COPYRIGHT 2005 ACS on STN

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

CN D-Glucose (8CI, 9CI) (CA INDEX NAME)
OTHER NAMES:
CN (+)-Glucose
CN Anhydrous dextrose
CN Cartose
CN Cerelose
CN Cerelose 2001
CN Clearsweet 95
CN Clintose L
CN Corn sugar
CN CPC hydrate
CN D(+)-Glucose
CN Dextropur
CN Dextrose
CN Dextrosol
CN Glucodin
CN Glucolin
CN Glucose

CN Glucosteril
CN Goldsugar
CN Grape sugar
CN Maxim Energy Gel
CN Meritose
CN Meritose 200
CN Roferose ST
CN Staleydex 111
CN Staleydex 130
CN Staleydex 333
CN Staleydex 95M
CN Sugar, grape
CN Tabfine 097(HS)
CN Vadex

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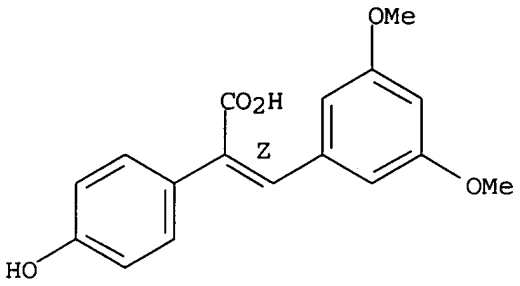
L2 ANSWER 1 OF 10 REGISTRY COPYRIGHT 2005 ACS on STN

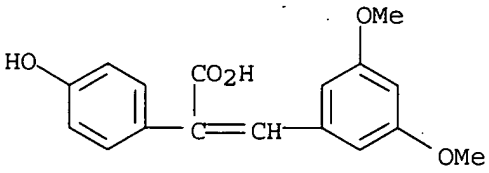
Double bond geometry as shown.



● Na

CN Benzeneacetic acid, α-[(3,5-dimethoxyphenyl)methylene]-4-hydroxy-, monosodium salt, (αZ)- (9CI) (CA INDEX NAME)

L2 ANSWER 2 OF 10 REGISTRY COPYRIGHT 2005 ACS on STN

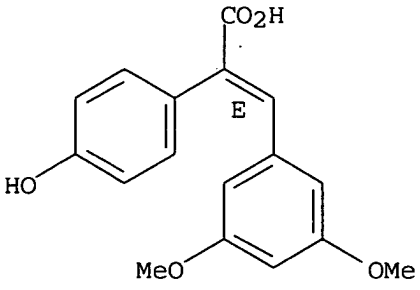


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

CN Benzeneacetic acid, α-[(3,5-dimethoxyphenyl)methylene]-4-hydroxy- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN 3-(3,5-Dimethoxyphenyl)-2-(4-hydroxyphenyl)acrylic acid
CN NSC 613734

L2 ANSWER 3 OF 10 REGISTRY COPYRIGHT 2005 ACS on STN

Double bond geometry as shown.

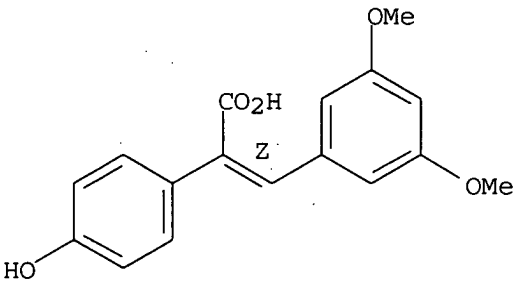


● Na

CN Benzeneacetic acid, α-[(3,5-dimethoxyphenyl)methylene]-4-hydroxy-, monosodium salt, (αE)- (9CI) (CA INDEX NAME)

L2 ANSWER 4 OF 10 REGISTRY COPYRIGHT 2005 ACS on STN

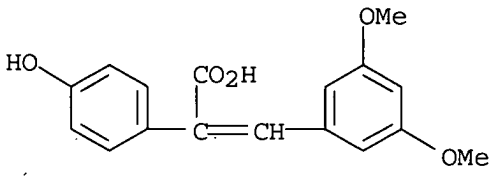
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

CN Benzeneacetic acid, α-[(3,5-dimethoxyphenyl)methylene]-4-hydroxy-, (αZ)- (9CI) (CA INDEX NAME)

L2 ANSWER 5 OF 10 REGISTRY COPYRIGHT 2005 ACS on STN



● Na

CN Benzeneacetic acid, α-[(3,5-dimethoxyphenyl)methylene]-4-hydroxy-, monosodium salt (9CI) (CA INDEX NAME)